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Comparison of the Growth of Pore and Shear Band Driven Detonations

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Abstract. We examine the effect of ignition site topology on the rate of reaction of a detonating material. The hot plane, hot line, and hot finite patch topologies are added to previous work on hot spot ignition. The hot plane and hot patch ignition forms would arise from ignition due to shear banding, and the hot line ignition form is shown to complete the topological set. The limiting behavior of instantaneous ignition is considered and used to construct simple reaction rate vs. extent of reaction forms. We fit simple form factor reaction rates, as might be available in most hydro codes with reactive flow modes, to the simple topologies. The difference between the rate vs. extent forms are examined with the objective that one should be able to use this information to distinguish between the different topological ignition forms.

Introduction

For secondary explosives, it has long been understood that some form of energy localization is required to get some fraction of the explosive hot enough to start a self propagating burn. This burn then progresses through the explosive, consuming that portion of the explosive that did not get heated hot enough from homogeneous shock to undergo rapid decomposition. The process of igniting the explosive is often known as the ignition phase, and the subsequent consumption phase is known as the growth and completion phase. One of the current controversies in detonation science is the nature of the ignition model. One hypothesis presumes that the ignition is driven by collapse of pores, where the explosive either forms a jet across the pore that effectively doubles the shock pressure on the far side of the pore, or collapses relatively uniformly with a high degree of viscous heating. Either form also heats any enclosed pore gases which heat up and could then lead to ignition by heating the surrounding explosive. The other hypothesis presumes that the ignition is driven by a shear banding processes that localizes the heat in a slip plane of the explosive crystal[1]. The energy is localized in a thin layer of explosive, creating an ignition sheet that then leads to simple laminar burn. Since these two mechanisms have significantly different geometrical signatures, there is a reasonable chance that one could distinguish between the two of them by the use of gauge records in a shock to detonation experiment.

In previous work we derived a statistical hot spot (SHS) model[2,3] for hot spot ignition and growth. The initial SHS model was based on the assumption that the ignition locations are hot spots that begin as a point or small sphere in space and then grow out. Initiation from a point is what is expected if the mechanism for initiation is driven by pore collapse, where the initial size of the hot spot is proportional the size of the initial pore. We also assumed that the location of these hot spots is randomly distributed throughout the system. From these simple assumptions and a laminar burn rate, one is able to develop a complete burn history without any further adjustable parameters. This has been verified in a recent paper by Hill et.al.[4]

In this paper, we extend that model to examine planar or sheet initiation, as one might expect from shear band ignition. We also include, for completeness, the possibility of ignition due to hot line, as one might expect about a line defect.

By integrating these two set of equations, it is possible to develop a $\dot{x}$ vs. x curve[5], where x is the extent of reaction, that can be compared to that of the hot spot mechanism. The differences between the hot spot and hot plane mechanisms can then be used to differentiate the growth and completion characteristics of shear band ignition from hot spot ignition.

Considerations of Basic Topology

There are a couple of cases to consider. The first, and simplest, is to assume that the shear band forms a sheet that is large enough to ignore edge effects. In this case, as we did before with the point ignition source, we develop a probability distribution for the amount of explosive that has not yet burned, based on the simple planar geometry. By use of a time differentiation, we construct a manifold of moment differential equations. Whereas the hot spot system consists of 5 equations, the hot plane system consists of only 3. The second case to consider is where the size of the shear band is not large enough to ignore the edge effects. In that case, we need to define an average patch size and initial perimeter length. The space that the expanding shear band occupies can then be decomposed into three different components – a plane of the initial area, a line of half the perimeter, and a single ignition point. Following the same derivation as used with the hot spot model, these terms separate, leading to probability of the explosive not being reacted that is a product of the planar, linear, and point ignition terms. As before, each of these geometries can be transformed into a differential manifold by differentiating them in time. Thus the final probability is developed from the product of three probabilities derived from these manifolds of 3, 4 and 5 linear differential equations, respectively.

Hot Planes

The hot plane analogy to the hot spot is as follows: Assume the existence of a single plane of combusted material in a volume V with an area A and that it has expanded R in both directions. The fraction of the total volume that this object occupies is just its volume divided by the total volume:

$$\frac{2RA}{V} \tag{1}$$

The probability that a point in space is not covered by the object, Q_1 is

$$Q_1 = 1 - \frac{2RA}{V} \cong \exp\left(-\frac{2RA}{V}\right), \tag{2}$$

where the second equality is the limit as the volume of the object is small compared to the total volume. In a real system, there will be several of these objects in any given volume. Assuming that the placement of these planes is uncorrelated, the probability of not being covered by any of them is then just the product of all of the individual Q probabilities. If we define $\rho_1(R,t)$ as the number density of planes with a given amount of expansion R, e. g. $\frac{n(R)A}{V}$, where $n(R)$ is the number in the volume, then we have the overall probability of not being covered as:

$$\mathrm{Q}_1(\mathrm{t}) = \exp\left(-\int_0^\infty dR\ 2R\rho_1(R,t)\right) \tag{3}$$

When we are considering hot spots, we particularly want to understand how they grow, so, as before, we will define the number density $\rho_1(\alpha,\omega)$ which is the number density of hot planes that are formed at time α and die at time ω. It is useful to note that $\rho_1(\alpha,\omega) = 0$ for $\alpha > \omega$ If we assume that the laminar burn rate of the hot plane ν is simply dependent on the current time, then

$$\rho_1(R,t) = \int_{-\infty}^{t} \left[\int_{t}^{\infty} \bar{\rho}_1(\alpha,\omega)\delta\left(R - \epsilon - \int_{\alpha}^{t} d\tau\, v(\tau)\right) d\omega + \int_{-\infty}^{t} \bar{\rho}_1(\alpha,\omega)\delta\left(R - \epsilon - \int_{\alpha}^{\omega} d\tau\, v(\tau)\right) d\omega \right] d\alpha, \tag{4}$$

where ϵ is the initial half thickness of the ignited plane. This integral states that the number density of planes is the sum of all planes that have been ignited and are still active, and those that have ignited and stopped reacting.

Let us make some definitions to simplify what follows:

$$f_1(t) \equiv 2\int_0^{\infty} dR\, R\rho_1(R,t) \tag{5}$$

The number of hot planes that have become active but could have died is

$$\rho_1(t) \equiv \int_{-\infty}^{t} \left[\int_{\alpha}^{\infty} \bar{\rho}_1(\alpha,\omega) d\omega\right] d\alpha. \tag{6}$$

The number of active planes is

$$\rho_1^A(t) \equiv \int_{-\infty}^{t} d\alpha\, \int_{t}^{\infty} d\omega\, \bar{\rho}_1(\alpha,\omega). \tag{7}$$

The rate of the number density of planes that became active at time t is:

$$\rho_1^B(t) = \int_{t}^{\infty} d\omega\, \bar{\rho}_1(t,\omega). \tag{8}$$

If we take the time derivative of f_1 we get

$$\frac{df_1(t)}{dt} = 2\epsilon\rho_1^B(t) + 2v(t)\rho_1^A(t) \tag{9}$$

$$\frac{d\rho_1^A(t)}{dt} = \rho_1^B(t) - \int_{-\infty}^{t} d\alpha\, \bar{\rho}_1(\alpha,t) \tag{10}$$

The second term in this last equation is the rate at which active hot sheets become inactive, or die. We call this the death rate. If the death rate is a fixed fraction μ_1 of the currently active hot sheets, then this last expression becomes

$$\frac{d\rho_1^A(t)}{dt} = \rho_1^B(t) - \mu_1\rho_1^A(t) \tag{11}$$

Hot lines

The hot line analogy to the hot spot is as follows: Assume the existence of a single line of combusted material in a volume V with a length L and that it has expanded R in both directions. The fraction of the total volume that this object occupies is just its volume divided by the total volume:

$$\frac{\pi R^2 L}{V} \tag{12}$$

The probability that a point in space is not covered by the object, Q, is

$$Q_2 = 1 - \frac{\pi R^2 L}{V} \cong \exp\left(-\frac{\pi R^2 L}{V}\right) \tag{13}$$

where the second equality is the limit as the volume of the object goes to zero. In a real system, there will be several of these objects in any given volume. Assuming that the placement of these lines is uncorrelated, the probability of not being covered by any of them is then just the product of all of the individual probabilities. If we define $\rho_2(R,t)$ as the number density of lines with a given radius R, e. g. $\frac{n(R)L}{V}$, where $n(R)$ is the number in the volume, then we have the overall probability of not being covered as:

$$\mathrm{Q_2(t)} = \exp\left(-\int_0^{\infty} dR\, \pi R^2 \rho_2(R,t)\right) \tag{14}$$

As before, when we want to understand how they grow, so we will define the number density $\rho_2(\alpha,\omega)$ which is the number density of hot lines that are formed at time α and die at time ω. If we assume that the growth rate ν of each hot line is simply dependent on the current time, then

$$\rho_2(R,t) = \int_{-\infty}^{t}\left[\int_{t}^{\infty}\bar{\rho}_2(\alpha,\omega)\delta\left(R-\epsilon-\int_{\alpha}^{t}d\tau\, v(\tau)\right)d\omega + \int_{-\infty}^{t}\bar{\rho}_2(\alpha,\omega)\delta\left(R-\epsilon-\int_{\alpha}^{\omega}d\tau\, v(\tau)\right)d\omega\right]d\alpha \tag{15}$$

Where ϵ is the initial half radius of the ignited line. This integral states that the number density of lines is the sum of all lines that have been ignited and are still active, and those that have ignited and stopped reacting.

Let us make some definitions to simplify what follows:

$$g_2(t) \equiv \pi \int_0^{\infty} dR\, R^2 \rho_2(R,t) \tag{16}$$

The number of hot lines that have become active but could have died is

$$\rho_2(t) \equiv \int_{-\infty}^{t}\left[\int_{\alpha}^{\infty}\bar{\rho}_2(\alpha,\omega)d\omega\right]d\alpha \tag{17}$$

The number of active planes is

$$\rho_2^A(t) \equiv \int_{-\infty}^{t} d\alpha\, \int_{t}^{\infty} d\omega\, \bar{\rho}_2(\alpha,\omega) \tag{18}$$

The number density of planes that became active at time t is:

$$\rho_2^B(t) = \int_{t}^{\infty} d\omega\, \bar{\rho}_2(t,\omega) \tag{19}$$

If we define

$$f_2^A(t) \equiv \int_0^{\infty} dR\, 2R \int_{-\infty}^{t}\left[\int_{t}^{\infty}\bar{\rho}_2(\alpha,\omega)\delta\left(R-\epsilon-\int_{\alpha}^{t}d\tau\, v(\tau)\right)d\omega\right]d\alpha \tag{20}$$

If the death rate is a fixed fraction μ of the currently active hot lines, then we have

$$\bar{\rho}_2(\alpha,t) = \mu \int_{t}^{\infty}\bar{\rho}_2(\alpha,\omega)d\omega \tag{21}$$

If we take the time derivative of g_2, f_2^A, ρ_2^A we have the following pde hierarchy:

$$\frac{dg_2(t)}{dt} = \pi\epsilon^2\rho_2^B(t) + \pi v(t) f_2^A(t) \tag{22}$$

$$\frac{df_2^A(t)}{dt} = 2\epsilon\rho_2^B(t) - \mu f_2^A(t) + 2v(t)\rho_2^A(t) \tag{23}$$

$$\frac{d\rho_2^A(t)}{dt} = \rho_2^B(t) - \mu\rho_2^A(t) \tag{24}$$

Finite Size Hot Planes

In a real system, it is unreasonable to assume that a planar ignition site will have infinite extent. For example, one does not field explosives that are made up of one single crystal. Thus, the size of the crystals in the explosive ensemble defines a maximum extent of hot plane. The ignition site of a hot plane can be defined by an average area A and perimeter length P. Using the concepts expressed in the previous sections, the fraction of the total volume subscribed by the hot patch is:

$$\frac{2RA+\frac{\pi}{2}R^2P+\frac{4\pi}{3}R^3}{V} \tag{25}$$

Thus, if the number density of patches with initial patch area A, initial perimeter P, and burned radius R is $\rho_p(A,P,R)$, then the probability of not being covered by one of these patches is just the product of the individual probabilities which equates integral over all of the patches:

$$Q_p(\mathrm{t}) = \exp\left(-\int_0^{\infty}\mathrm{dA}\,\int_0^{\infty}\mathrm{dP}\int_0^{\infty}\mathrm{dR}\,\rho_p(\mathrm{A,P,R,t})\left[2\mathrm{RA}+\frac{\pi}{2}\mathrm{R}^2\mathrm{P}+\frac{4\pi}{3}\mathrm{R}^3\right]\right) \tag{26}$$

Note, by making the assumption that the volume of any given hot spot is small compared to the total volume, we can neglect the fact that it is impossible for the perimeter of the hot patch to burn any other part of the same patch, as this overlap would be vanishingly small. Thus, Q_p can be broken into the planar, line, and point components that we have already described, either in this paper or previous ones. One can now integrate each component over A and P, and then write the equation in terms of the average area $\bar{A}$ and average perimeter length $\bar{P}$.

$$Q_p(\mathrm{t}) = \exp\left(-\int_0^\infty \mathrm{dR}\,\rho_p(\mathrm{R},\mathrm{t})\left[2\mathrm{R}\bar{A} + \frac{\pi}{2}\mathrm{R}^2\bar{\mathrm{P}} + \frac{4\pi}{3}\mathrm{R}^3\right]\right) \tag{27}$$

Let us define the following relations to reduce the complexity of these equations: $\bar{A} = \alpha\left(\frac{\bar{P}}{4}\right)^2$. If the patch is a circle, $\alpha = 4/\pi$, and if it is a square it is 1. Similarly, let us define $R = \left(\left(\frac{\bar{P}}{4}\right)r\right)$, and $\beta(r,t)dr = \left(\frac{\bar{P}}{4}\right)^3 \rho_P(R,t)dR$. With these definitions, the probability of not having burned is just

$$(1-\mathrm{x(t)}) = \exp\left(-2\int_0^\infty dr\beta(r,t)\left[\alpha r + \pi\mathrm{r}^2 + \frac{2\pi}{3}\mathrm{r}^3\right]\right) \tag{28}$$

It is interesting to note that even with the complexity of a finite sized patch, we are still left with only two parameters – the patch geometry and the overall density of patches. As before, the density of hot patches will be defined as an integral over the ignition and death time of the individual hot patches, replacing ρ_p with β.

Limits of Instantaneous Ignition and Uniform Burn Rate

Let us examine the behavior if $\rho_2(\alpha,\omega) = \rho_2\delta(t-\alpha)$ and $\nu(t) = \nu$. This implies the $\mu = 0$ and $\rho_2^B(t) = \rho\delta(t-\alpha)$. So the probability of not being reacted is then just

$$Q_2(t) = (1-x_2) = \begin{cases} e^{-\pi\rho_2(\epsilon+(t-\alpha)\nu)^2} & t > \alpha \\ 1 & t \le \alpha \end{cases} \tag{29}$$

Let us now compute $\dot{x}_2(x_2)$:

$$x_2 = 1 - e^{-\pi\rho_2(\epsilon+(t-\alpha)\nu)^2} \tag{30}$$

$$\dot{x}_2 = 2(\pi\rho_2)^{\frac{1}{2}}\nu(1-x_2)(-\ln(1-x_2))^{\frac{1}{2}} \tag{31}$$

The same reasoning can be applied to each of the simple 1, 2, and 3 dimensional ignition forms. If we define a normalized burn velocity G_n for each dimension, we find we can write the $\dot{x}_n(x_n)$ function as

$$\dot{x}_n = nG_n(1-x_n)[-\ln(1-x_n)]^{\frac{n-1}{n}} \tag{32}$$

In principle, this expression could be used to determine the effective dimensionality of the ignition surface. We list the value of G_n in table 1

It is typical for codes that implement reactive flow models to have a growth/completion model based on what is known as a form factor reaction: $\dot{x} = Fx^\eta(1-x)^\zeta$. To aid rapid implementation of these models, we provide fits to that form in Table 1. In table 1 we show both the unconstrained fits (the first line of the table for a particular geometry) and the fit that is constrained to exactly match the early time behavior.

Now let us consider this limit for the finite sized patch. The derivative of mass fraction is just

$$\dot{x} = \beta\dot{r}(1-x)[2\alpha + 4\pi r + 4\pi r^2] \tag{33}$$

Here, r is short hand for $4(\epsilon + (t-\alpha)\nu)/\bar{P}$. In order to get this in the form of $\dot{x}(x)$, we need to solve the following cubic equation for r as a function of x.

$$0 = \frac{4\pi}{3}\beta r^3 + 2\pi\beta r^2 + 2\alpha\beta r + \ln(1-x) \tag{34}$$

Table 1: Effective form factor parameters and normalized burn velocity of the three basic hot spot geometries. Where two lines are present for a given geometry, the second parameterization enforces that the early time behavior is exact.

Ignition Source	F	η	ζ	**RMS Error**	G_n
Hot plane	G_1	0	1	0	$2\nu\rho_1$
Hot line	$2.08067\ G_2$	0.515439	0.807104	0.003139	$\nu(\pi\rho_2)^{\frac{1}{2}}$
	$2.0\ G_2$	0.5	0.777561	0.007147	
Hot spot	$3.203796\ G_3$	0.695014	0.751105	0.006139	$\nu\left(\frac{4\pi\rho_3}{3}\right)^{\frac{1}{3}}$
	$3.0\ G_3$	0.66667	0.706635	0.015391	

The solution of the cubic equation is straight forward.

Results

We compare the rate expressions for the three different basic configurations in figure 1. Clearly, as the dimensionality of the ignition size increases (from a plane to a point), the maximum rate moves to points with higher extent of reaction.

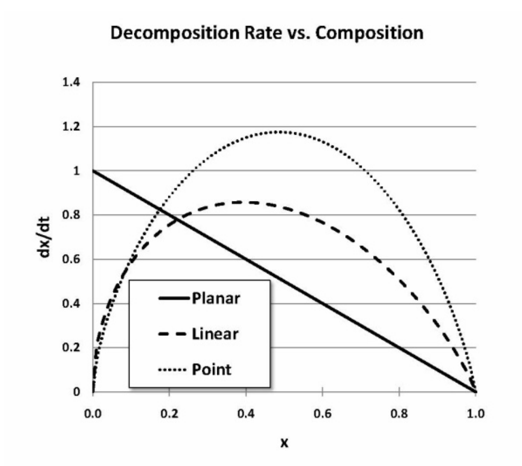

Fig 1: Decomposition rate as a function of composition for the three basic ignition forms.

Let us now consider the finite sized patch system. In figure 2 we show the rate expressions, normalized to the maximum value over the range of x, for the finite size patch with $\alpha = 4/\pi$, and varying β from 0.01 to 100. The chosen value of α corresponds to igniting a round patch of explosive. Large values of β indicate that a large amount of material is being ignited for each ignition site, while small values of β indicate that the area of the hot patch is isolated or sparse. Figure 2 shows that for round hot patches, the normalized rate for small values of β acts like a hot spot, while large values act like a hot plane. In essence, large values of β indicate that the explosive material will be consumed before the edge effects have a chance to modify the reaction behavior.

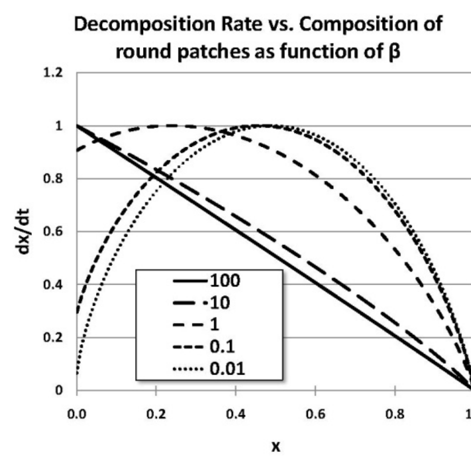

Fig 2. Normalized decomposition rate as a function of composition for the finite round ($\alpha = 4/\pi$) ignition patch β varying from 0.01 to 100.

In Figure 3 we consider the case with $\alpha = 1/3$ as a function of β. Again, we are holding the topology of the patch fixed as we change the density of these hot patches. This value of α roughly corresponds to a rectangular patch with width approximately 10% of the length. As before, as β gets smaller, the hot patch becomes more hot spot like. This corresponds to the fact that the hot patch does not encompass a large volume of space, so that over time the mere existence of the finite size washes out the initial shape of the patch. As β gets larger, the shape of the initial hot patch starts to dominate the reaction rate.

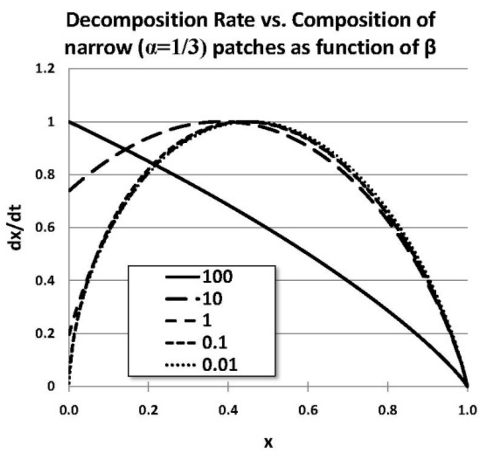

Fig 3. Normalized decomposition rate as a function of composition for the finite ignition patch with $\alpha = 1/3$ and β varying from 0.01 to 100.

Finally, in Figure 4 we examine the effect of α on the shape of the decomposition rate curve. As α goes from $4/\pi$ to 0, we start with a single round hot patch inside an roughly spherical crystal ($\alpha = 4/\pi$), to a square patch in a cubic crystal ($\alpha = 1$), and go to either 8 line segment patches in a cubic crystal or 4 line segments through a spherical crystal ($\alpha = 0$). It is interesting to note that the peak of the $\dot{x}$ curve is not monotonically increasing with decreasing α. In fact, the largest extent of reaction that corresponds to a maximum reaction rate is 0.45 which occurs when $\alpha \sim 0.4$ for $\beta = 1$. This is roughly halfway between the extent of reaction of the maximum reaction rate for the hot point and hot line hot spots.

Since the location of the maximum reaction rate is a non-monotonic function, it becomes obvious that discriminating between different topologies cannot be done by simply noting the point of maximum reaction rate. Essentially, we find that a peak rate at low extent of reaction can be ascribed to either thin line-like ignition zones, or relatively small planar patches. The telltale difference between these two ignition topologies is the initial reaction rate. The initial reaction rate is directly related to the extent that the ignition mechanism ignites planar sheets. Thus, though these different topologies may peak at the same point, planar based topologies will have an initially faster reaction.

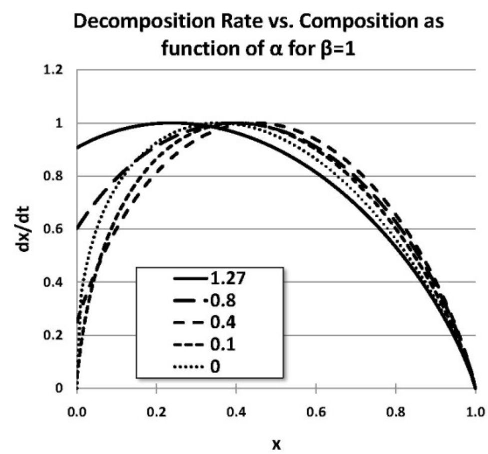

Fig 4. Normalized decomposition rate as a function of α for $\beta = 1$. Note that the peak location is not monotonically varying with α.

Conclusions

In this paper we have examined the effect of different ignition topologies on the geometric reaction rate of detonating high explosives. By making some simplifying assumptions on the intrinsic rate expressions, we were able to derive the reaction form factors of detonating high explosives that one could use in a standard hydro code.

The detonation process can be a rather complex combination of effects. The reaction mechanisms discussed here apply to the initial conversion from solid explosive to gas due to a heterogeneous reaction mechanism (hot spots or shear bands). To the extent that the detonation reaction is being driven by either slow reactions, as in carbon-cluster formation, or homogeneous solid decomposition reactions due to the adiabatic heating of the explosive, the behaviors derived here will be obscured.

With those caveats in mind, however, one should be able to use the reaction rate forms derived here to differentiate between explosives driven by hot spot ignition/initiation and those driven by shear banding. In order to do this, one needs the equation of state of the reactant and product species, pressure traces from the von Neumann spike to the state where the solid is no longer burning, which is often the CJ state, and the burn rate of the explosive. By calculating the equilibrium pressure along the Rayleigh line, one can back out the extent of reaction as a function of time. One can then construct the rate vs. extent of reaction curve that can be compared to these reaction forms.

Acknowledgements

The author would like to thank Craig Tarver for useful discussions as this model was being developed. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Discussion

Question, David Dunlap, UNM:

In diffusion-limited capture by randomly placed traps people are sometimes interested in the long-time tails of the survival probability. At early times there is an exponential decay of the probability, but at long times what is left to be captured "lives on" in relatively trap-free voids (like your pores), the size of these sparse regions governed by the Poisson distribution function. This modifies the long time behavior, such that the tail of the survival probability is a slower-than-exponential decay going as exp(-t^(d/(d+2)) where d is the dimensionality. There is a reference, M. D. Donsder and SRS Varadhan, Commun. Pure Appl. Math 28 (1975) p.525 to which this is attributed.

So when I was listening to your talk, and saw you attributing the consumption rate to the distribution of pore sizes, I was struck by the possible similarity of your analysis and this. I hope this is helpful.

Reply by A. Nichols:

It is typical for reactive flow models to construct something which has a finite completion time. This helps in several issues in a hydro code. The point I am making, and your references corroborate, is that the completion rate of the hot spots is NOT simple and not over a finite time. Thus these simple models have a fundamental flaw in their long time behavior that is resolved with the statistical hot spot models.